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Table 1.2.13.1. *General reflection conditions due to glide planes and screw axes*

(*a*) Layer groups.
(1) Glide planes.

Reflection condition	Orientation of plane	Glide vector	Symbol
hk: $h = 2n$	(001)	**a**/2	*a*
hk: $k = 2n$	(001)	**b**/2	*b*
hk: $h + k = 2n$	(001)	**a**/2 + **b**/2	*n*
$0k$: $k = 2n$	(100)	**b**/2	*b*
$h0$: $h = 2n$	(010)	**a**/2	*a*

(2) Screw axes.

Reflection condition	Direction of axis	Screw vector	Symbol
$h0$: $h = 2n$	[100]	**a**/2	2_1
$0k$: $k = 2n$	[010]	**b**/2	2_1

(*b*) Rod groups.
(1) Glide planes.

Reflection condition	Orientation of plane	Glide vector	Symbol
l: $l = 2n$	Any orientation parallel to the *c* axis	**c**/2	*c*

(2) Screw axes.

Reflection condition	Direction of axis	Screw vector	Symbol
l: $l = 2n$	[001]	**c**/2	2_1, 4_2, 6_3
l: $l = 3n$	[001]	**c**/3	3_1, 3_2, 6_2, 6_4
l: $l = 4n$	[001]	**c**/4	4_1, 4_3
l: $l = 6n$	[001]	**c**/6	6_1, 6_5

(*c*) Frieze groups, glide plane.

Reflection condition	Orientation of plane	Glide vector	Symbol
h: $h = 2n$	(10)	**a**/2	*g*

the site-symmetry group belongs to a lower crystal system. For example, for the 2*c* position of tetragonal layer group *p*4*mm* (L55), the site-symmetry group is the orthorhombic group '2*mm*.'. The two characters '*mm*' represent the secondary set of tetragonal symmetry directions, whereas the dot represents the tertiary tetragonal symmetry direction.

1.2.13. Reflection conditions

The *Reflection conditions* are listed in the right-hand column of each Wyckoff position. There are two types of reflection conditions:

(i) *General conditions*. These conditions apply to *all* Wyckoff positions of the subperiodic group.

(ii) *Special conditions* ('extra' conditions). These conditions apply only to *special* Wyckoff positions and must always be added to the general conditions of the subperiodic group.

The *general reflection conditions* are the result of three effects: centred lattices, glide planes and screw axes. For the nine layer groups with *centred* lattices, the corresponding general reflection condition is $h + k = 2n$. The general reflection conditions due to glide planes and screw axes for the subperiodic groups are given in Table 1.2.13.1.

Example: The layer group p4bm (L56)

General position 8*d*: $0k: k = 2n$ and $h0: h = 2n$ due respectively to the glide planes *b* and *a*. The projections along [100] and [010] of any crystal structure with this layer-group symmetry have, respectively, periodicity **b**/2 and **a**/2.

Special positions 2*a* and 2*b*: $hk: h + k = 2n$. Any set of equivalent atoms in either of these positions displays additional *c*-centring.

1.2.14. Symmetry of special projections

1.2.14.1. Data listed in the subperiodic group tables

Under the heading *Symmetry of special projections*, the following data are listed for three orthogonal projections of each layer group and rod group and two orthogonal projections of each frieze group:

(i) For layer and rod groups, each projection is made onto a plane normal to the projection direction. If there are three kinds of symmetry directions (*cf.* Table 1.2.4.1), the three projection directions correspond to the primary, secondary and tertiary symmetry directions. If there are fewer than three symmetry directions, the additional projection direction(s) are taken along coordinate axes.

For frieze groups, each projection is made on a line normal to the projection direction.

The directions for which data are listed are as follows:

(*a*) *Layer groups*:

Triclinic/oblique Monoclinic/oblique Monoclinic/rectangular Orthorhombic/rectangular	[001], [100], [010]
Tetragonal/square	[001], [100], [110]
Trigonal/hexagonal Hexagonal/hexagonal	[001], [100], [210]

(*b*) *Rod groups*:

Triclinic Monoclinic/inclined Monoclinic/orthogonal Orthorhombic	[001], [100], [010]
Tetragonal	[001], [100], [110]
Trigonal Hexagonal	[001], [100], [210]

(*c*) *Frieze groups*:

Oblique Rectangular	[10], [01]

(ii) *The Hermann–Mauguin symbol*. For the [001] projection of a layer group, the Hermann–Mauguin symbol for the plane group resulting from the projection of the layer group is given. For the [001] projection of a rod group, the Hermann–Mauguin symbol for the resulting two-dimensional point group is given. For the remainder of the projections, in the case of both layer groups and

Table 1.2.14.1. *a', b', γ' (a') of the projected conventional coordinate system in terms of a, b, c, α, β, γ (a, b, γ) of the conventional coordinate system of the layer and rod groups (frieze groups)*

(*a*) Layer groups.

Projection direction	Triclinic/oblique	Monoclinic/oblique
[001]	$a' = a\sin\beta$ $b' = b\sin\alpha$ $\gamma' = 180^\circ - \gamma^*$†	$a' = a$ $b' = b$ $\gamma' = \gamma$
[100]	$a' = b\sin\gamma$ $b' = c\sin\beta$ $\gamma' = 180^\circ - \alpha^*$†	$a' = b\sin\gamma$ $b' = c$ $\gamma' = 90^\circ$
[010]	$a' = a\sin\gamma$ $b' = c\sin\alpha$ $\gamma' = 180^\circ - \beta^*$†	$a' = a\sin\gamma$ $b' = c$ $\gamma' = 90^\circ$
	Monoclinic/ rectangular	Orthorhombic/ rectangular
[001]	$a' = a$ $b' = b\sin\alpha$ $\gamma' = 90^\circ$	$a' = a$ $b' = b$ $\gamma' = 90^\circ$
[100]	$a' = b$ $b' = c$ $\gamma' = \alpha$	$a' = b$ $b' = c$ $\gamma' = 90^\circ$
[010]	$a' = a$ $b' = c\sin\alpha$ $\gamma' = 90^\circ$	$a' = a$ $b' = c$ $\gamma' = 90^\circ$
	Tetragonal/square	
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$	
[100]	$a' = a$ $b' = c$ $\gamma' = 90^\circ$	
[110]	$a' = (a/2)(2)^{1/2}$ $b' = c$ $\gamma' = 90^\circ$	
	Trigonal/hexagonal, hexagonal/hexagonal	
[001]	$a' = a$ $b' = a$ $\gamma' = 120^\circ$	
[100]	$a' = [(3)^{1/2}/2]a$ $b' = c$ $\gamma' = 90^\circ$	
[210]	$a' = a/2$ $b' = c$ $\gamma' = 90^\circ$	

† $\cos\alpha^* = (\cos\beta\cos\gamma - \cos\alpha)/(\sin\beta\sin\gamma)$,
$\cos\beta^* = (\cos\gamma\cos\alpha - \cos\beta)/(\sin\gamma\sin\alpha)$,
$\cos\gamma^* = (\cos\alpha\cos\beta - \cos\gamma)/(\sin\alpha\sin\beta)$.

(*b*) Rod groups.

Projection direction	Triclinic	Monoclinic/inclined
[001]	$a' = a\sin\beta$ $b' = b\sin\alpha$ $\gamma' = 180^\circ - \gamma^*$†	$a' = a$ $b' = b\sin\alpha$ $\gamma' = 90^\circ$
[100]	$a' = c\sin\beta$ $b' = b\sin\gamma$ $\gamma' = 180^\circ - \alpha^*$†	$a' = c$ $b' = b$ $\gamma = \alpha$
[010]	$a' = c\sin\alpha$ $b' = a\sin\gamma$ $\gamma' = 180^\circ - \beta^*$†	$a' = c\sin\alpha$ $b' = a$ $\gamma' = 90^\circ$
	Monoclinic/ orthogonal	Orthorhombic
[001]	$a' = a$ $b' = b$ $\gamma' = \gamma$	$a' = a$ $b' = b$ $\gamma' = 90^\circ$
[100]	$a' = c$ $b' = b\sin\gamma$ $\gamma' = 90^\circ$	$a' = c$ $b' = b$ $\gamma' = 90^\circ$
[010]	$a' = c$ $b' = a\sin\gamma$ $\gamma' = 90^\circ$	$a' = c$ $b' = a$ $\gamma' = 90^\circ$
	Tetragonal	
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$	
[100]	$a' = c$ $b' = a$ $\gamma' = 90^\circ$	
[110]	$a' = c$ $b' = (a/2)(2)^{1/2}$ $\gamma' = 90^\circ$	
	Trigonal, hexagonal	
[001]	$a' = a$ $b' = a$ $\gamma' = 120^\circ$	
[100]	$a' = c$ $b' = [(3)^{1/2}/2]a$ $\gamma' = 90^\circ$	
[210]	$a' = c$ $b' = a/2$ $\gamma' = 90^\circ$	

(*c*) Frieze groups.

Projection direction	Oblique	Rectangular
[10]	$a' = b\sin\gamma$	$a' = b$
[01]	$a' = a\sin\gamma$	$a' = a$

rod groups, the Hermann–Mauguin symbol is given for the resulting frieze group. For the [10] projection of a frieze group, the Hermann–Mauguin symbol of the resulting one-dimensional point group, *i.e.* 1 or *m*, is given. For the [01] projection, the Hermann–Mauguin symbol of the resulting one-dimensional space group, *i.e.* *p*1 or *pm*, is given.

(iii) For layer groups, the basis vectors $\mathbf{a}'$, $\mathbf{b}'$ of the plane group resulting from the [001] projection and the basis vector $\mathbf{a}'$ of the frieze groups resulting from the additional two projections are given as linear combinations of the basis vectors $\mathbf{a}$, $\mathbf{b}$ of the layer group. Basis vectors $\mathbf{a}$, $\mathbf{b}$ inclined to the plane of projection are replaced by the projected vectors $\mathbf{a}_p$, $\mathbf{b}_p$. For the two projections of a rod group resulting in a frieze group, the basis vector $\mathbf{a}'$ of the resulting frieze group is given in terms of the basis vector $\mathbf{c}$ of the rod group. For the [01] projection of a frieze group, the basis vector $\mathbf{a}'$ of the resulting one-dimensional space group is given in terms of the basis vector $\mathbf{a}$ of the frieze group.

For rod groups and layer groups, the relations between a', b' and γ' of the projected conventional basis vectors and a, b, c, α, β and γ of the conventional basis vectors of the subperiodic group are given in Table 1.2.14.1. We also give in this table the relations between a' of the projected conventional basis and a, b and γ of the conventional basis of the frieze group.

Table 1.2.14.2. *Projection of three-dimensional symmetry elements (layer and rod groups)*

Symmetry element in three dimensions		Symmetry element in projection	
Arbitrary orientation			
Symmetry centre $\bar{1}$		Rotation point 2 at projection of centre	
Parallel to projection direction			
Rotation axis	2, 3, 4, 6	Rotation point	2, 3, 4, 6
Screw axis	2_1	Rotation point	2
	3_1, 3_2		3
	4_1, 4_2, 4_3		4
	6_1, 6_2, 6_3, 6_4, 6_5		6
Rotoinversion axis	$\bar{4}$	Rotation point	4
	$\bar{6} \equiv 3/m$		3 (with overlap of atoms)
	$\bar{3} \equiv 3 \times \bar{1}$		6
Reflection plane *m*		Reflection line *m*	
Glide plane with ⊥ component†		Glide line *g*	
Glide plane without ⊥ component†		Reflection line *m*	
Normal to projection direction			
Rotation axis	2, 4, 6	Reflection line *m*	
	3	None	
Screw axis	4_2, 6_2, 6_4	Reflection line *m*	
	2_1, 4_1, 4_3, 6_1, 6_3, 6_5	Glide line *g*	
	3_1, 3_2	None	
Rotoinversion axis	$\bar{4}$	Reflection line *m* parallel to axis	
	$\bar{6} \equiv 3/m$	Reflection line *m* perpendicular to axis	
	$\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)	
Reflection plane *m*		None, but overlap of atoms	
Glide plane with glide component **t**		Translation **t**	

† The term 'with ⊥ component' refers to the component of the glide vector normal to the projection direction.

(iv) *Location of the origin* of the plane group, frieze group and one-dimensional space group is given with respect to the conventional lattice of the subperiodic group. The same description is used as for the location of symmetry elements (see Section 1.2.9). *Example*: 'Origin at *x*, 0, 0' or 'Origin at *x*, 1/4, 0'.

1.2.14.2. *Projections of centred subperiodic groups*

The only centred subperiodic groups are the nine types of centred layer groups. For the [100] and [010] projection directions, because of the centred layer-group lattice, the basis vectors of the resulting frieze groups are $\mathbf{a}' = \mathbf{b}/2$ and $\mathbf{a}' = \mathbf{a}/2$, respectively.

1.2.14.3. *Projection of symmetry elements*

A symmetry element of a subperiodic group projects as a symmetry element only if its orientation bears a special relationship to the projection direction. In Table 1.2.14.2, the three-dimensional symmetry elements of the layer and rod groups and in Table 1.2.14.3 the two-dimensional symmetry elements of the frieze groups are listed along with the corresponding symmetry element in projection.

Example: Layer group cm2m (L35)

Projection along [001]: This orthorhombic/rectangular plane group is centred; *m* perpendicular to [100] is projected as a reflection line, 2 parallel to [010] is projected as the same reflection line and *m* perpendicular to [001] gives rise to no symmetry element in projection, but to an overlap of atoms. *Result*: Plane group *c*1*m*1 (5) with $\mathbf{a}' = \mathbf{a}$ and $\mathbf{b}' = \mathbf{b}$.

Projection along [100]: The frieze group has the basis vector $\mathbf{a}' = \mathbf{b}/2$ due to the centred lattice of the layer group. *m* perpendicular to [100] gives rise only to an overlap of atoms, 2 parallel to [010] is projected as a reflection line and *m* perpendicular to [001] is projected as the same reflection line. *Result*: Frieze group $\not{p}11m$ (F4) with $\mathbf{a}' = \mathbf{b}/2$.

Projection along [010]: The frieze group has the basis vector $\mathbf{a}' = \mathbf{a}/2$ due to the centred lattice of the layer group. The two reflection planes project as perpendicular reflection lines and 2 parallel to [010] projects as the rotation point 2. *Result*: Frieze group $\not{p}2mm$ (F6) with $\mathbf{a}' = \mathbf{a}/2$.

1.2.15. Maximal subgroups and minimal supergroups

In *IT* A (2005), for the representative space group of each space-group type the following information is given:

(i) maximal non-isomorphic subgroups,
(ii) maximal isomorphic subgroups of lowest index,
(iii) minimal non-isomorphic supergroups and
(iv) minimal isomorphic supergroups of lowest index.

However, Bieberbach's theorem for space groups, *i.e.* the classification into isomorphism classes is identical with the classification into affine equivalence classes, is not valid for subperiodic groups. Consequently, to obtain analogous tables for the subperiodic groups, we provide the following information for each representative subperiodic group:

(i) maximal non-isotypic non-enantiomorphic subgroups,
(ii) maximal isotypic subgroups and enantiomorphic subgroups of lowest index,